AEC RESEARCH AND
DEVELOPMENT REPORT

NEW YORK UNIVERSITY

institute of mathematical sciences

AEC Computing Facility

New York, New York

NYO-6480
PHYSICS

STEADY STATES, BOUNDEDNESS, AND NUMERICAL ANALYSIS OF TEMPERATURE AND NEUTRON DENSITY IN CIRCULATING FUEL REACTORS

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CONTRACT NO. AT(30-1)-1480

July 1, 1955

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ABSTRACT

A system of non-linear partial differential equations for the neutron density and temperature in a circulating fuel reactor is studied. A steady-state solution of these equations is obtained together with conditions which guarantee its existence and uniqueness. Further conditions are obtained which are sufficient to insure the boundedness of the temperature for all time. Explicit bounds are obtained when the excess multiplication factor is a linear function of temperature.

A numerical method for the solution of the non-linear equations is presented. This procedure is shown to be stable and convergent under stated conditions on the mesh.

Section 1. Introduction

A system of non-linear partial differential equations for the thermal neutron density and temperature in a circulating fuel reactor has been derived and studied by Dr. J. Fleck [1] of the Brookhaven National Laboratory. In the derivation, which is summarized in section 2, the excess multiplication factor, k_{ex}, is taken to be a linear function of the temperature V. The present report considers a general, unspecified, dependence of k_{ex} on temperature.

In section 3 sufficient conditions are obtained on the function $k_{ex}(V)$ to guarantee the existence of non-trivial steady state solutions. Additional conditions are stated which are sufficient to insure that a non-constant steady state is unique. The steady state temperature and neutron density are given implicitly in terms of integrals of $k_{ex}(V)$. These results are applied, as an example, to the special case assumed in [1]. Here a bound on the steady state exit temperature is obtained in terms of the input temperature.

In section 4 the question of boundedness of the temperature for all time is considered. A relatively weak condition on $k_{ex}(V)$ is shown to be sufficient to insure that the temperature remain between specified bounds which depend on the initial and boundary data and the form of the function $k_{ex}(V)$. In the case of the linear temperature dependence, assumed in [1], which always satisfies the required condition for

boundedness, explicit bounds are obtained.

A method for the numerical computation of the temperature and neutron density is presented in Section 5. The conditions for stability and an estimate of the error in this scheme are examined in Section 6. A discussion of some of the numerical results which have been obtained with the use of this method is to be included in [1].

Section 2. Formulation

Let a cylindrical circulating fuel reactor with axis parallel to the X-axis occupy the range $0 \leq X \leq A$. The thermal neutron density may be taken as $U(T, X)R(y, z)$, where R satisfies

(2.1)
$$R_{yy} + R_{zz} + (B^2-\beta^2)R = 0 \quad ,$$
$$R(y, z) = 0 \quad , \text{ for } (y, z) \text{ on the cylindrical surface;}$$

and $U(T, X)$ satisfies

(2.2)
$$\ell U_T = h^2(U_{xx} + \beta^2 U) + [k_{eff}-1]U$$ [redacted] ,
$$U(T, 0) = U(T, A) = 0 \quad .$$

Here we have used the notation

$\ell_o \equiv$ thermal neutron lifetime , $\beta \equiv \pi/A$,

$L \equiv$ thermal diffusion length , $\ell \equiv \ell_o/1+L^2B^2$,

(2.3) $k \equiv$ infinite reactor multiplication, $h^2 \equiv L^2/1+L^2B^2$,

$\tau \equiv$ Fermi age of thermal neutrons , $k_{eff} \equiv ke^{-B^2\tau}/1+L^2B^2$,

$B^2 \equiv$ reactor buckling.

If the fuel is flowing with constant velocity $C > o$ in the positive X-direction, its temperature, given by $V(T, X)R(y, z)$, must satisfy

$$(2.4) \qquad \begin{aligned} &V_T + CV_X = U \\ &V(T, o) = V_o \quad . \end{aligned}$$

Here V_o is the constant input temperature and the units are appropriately chosen such that temperature is measured in ^{o}C. It is assumed that the significant effects of temperature on the reactor kinetics may be obtained by taking the excess multiplication factor, $[k_{eff}-1] \equiv k_{ex}$, to be a given function of temperature; say

$$(2.5) \qquad [k_{eff}-1] = \varepsilon-\delta V \quad ,$$

with $\varepsilon, \delta > o$. Equations (2.2), (2.4) and (2.5) may be written in dimensionless form as

$$(2.6) \qquad \begin{aligned} &a)\ u_t = u_{xx} + [1-v]u \\ &b)\ v_t + cv_x = u \quad , \end{aligned}$$

with the boundary conditions

$$(2.7) \qquad \begin{aligned} &a)\ u(t, o) = u(t, a) = 0 \\ &b)\ v(t, o) = v_o \quad . \end{aligned}$$

The dimensionless variables are defined by

$$(2.8) \qquad \begin{aligned} &t = {}^{p^2}/_{\ell}\, T \quad , \qquad x = {}^{p}/_{h}\, X \quad , \qquad c = {}^{\ell}/_{ph}\, C \\ &u = \frac{\ell\delta}{p^4}\, U \quad , \qquad v = {}^{\delta}/_{p^2}\, V \quad , \qquad \text{where } p^2 = \varepsilon + \beta^2 h^2 \quad , \end{aligned}$$

and a and v_o are the dimensionless length and input temperature respectively. Equations (2.1) - (2.8) are a summary of the formulation derived in [1].

The temperature dependence assumed in (2.5) simplifies analytical attempts to investigate the resulting system of equations. It also assures a negative temperature coefficient of reactivity for all positive temperatures which, at least intuitively, seems sufficient to prevent unbounded temperatures and neutron densities. That this is so for the temperature, is shown as an example in Section 4. However it is important to know what general types of dependence of k_{ex} on V lead to bounded temperatures. Thus we take

$$(2.9) \qquad [k_{eff}-1] = k_{ex}(V) \quad ,$$

where the functional form is unspecified and we are not restricted to negative temperature coefficients. Introducing variables analogous to those of (2.8), but not necessarily dimensionless, equations (2.2), (2.4) and (2.9) become

$$(2.10) \qquad \begin{aligned} &a) \quad u_t = u_{xx} + A(v)u \\ &b) \quad v_t + cv_x = u \quad , \end{aligned}$$

with the boundary conditions (2.7). The restrictions imposed on $k_{ex}(V)$ are given in Sections 3 and 4 as conditions on A(v). They are shown to be satisfied for A(v) = 1 -v.

To complete the formulation we specify the initial conditions

$$(2.11) \qquad \begin{aligned} &a) \quad u(o, x) = f(x) \\ &b) \quad v(o, x) = g(x) \quad , \end{aligned}$$

where, since u is a density, we require

$$(2.12) \quad f(x) \geq o \quad , \quad o \leq x \leq a \quad .$$

In order to avoid the consideration of discontinuities we also require

$$(2.13) \quad g(o) = v_o \quad ,$$

and assume that all functions introduced have continuous derivatives of at least fourth order.

Section 3. The Steady State

Let the steady state be described by the variables

$$(3.1) \quad \begin{aligned} u(x) &= \lim_{t \to \infty} u(t, x) \\ v(x) &= \lim_{t \to \infty} v(t, x) \quad . \end{aligned}$$

This notation will be used only in the present section and to avoid confusion the arguments (t, x) shall be included for all non-steady-state quantities. With the assumption that $\lim_{t \to \infty} u_t(t, x) = \lim_{t \to \infty} v_t(t, x) = 0$, we obtain from (2.10)

$$(3.2) \quad \begin{aligned} &a) \quad u'' + A(v)u = 0 \\ &b) \quad cv' = u \quad . \end{aligned}$$

The boundary conditions are, from (2.7)

$$(3.3) \quad \begin{aligned} &a) \quad u(o) = u(a) = 0 \\ &b) \quad v(o) = v_o \quad . \end{aligned}$$

In Section 4 it is shown that $u(t, x) \geq o$ for all $t \geq o$. Anticipating this result we require

$$(3.4) \qquad u(x) \geq o \quad , \quad o \leq x \leq a \quad .$$

One solution of the above equations is the constant steady state: $u = o$, $v = v_o$. We consider this to be a trivial solution and seek other non-trivial steady states.

Some qualitative features of non-trivial solutions are immediate consequences of (3.2b), (3.3a) and (3.4). They imply that $v(x)$ must be a monotonic increasing function of x with horizontal slope at $x = o$ and $x = a$. For a complete analysis we introduce the quantities

$$(3.5) \qquad v_e \equiv v(a), \text{ the exit temperature;}$$

$$(3.6) \qquad B(v, v_o) \equiv \int_{v_o}^{v} A(\xi)d\xi \quad ;$$

$$(3.7) \qquad C(v, v_o) \equiv \int_{v_o}^{v} B(\xi, v_o)d\xi \quad ;$$

$$(3.8) I(v; v_e, v_o) \equiv \left[\frac{v_e - v_o}{2}\right]^{1/2} \int_{v_o}^{v} \left[(\xi - v_o)C(v_e, v_o) - (v_e - v_o)C(\xi, v_o)\right]^{-1/2} d\xi .$$

Eliminating u in (3.2), integrating the resulting differential equation, and applying the boundary conditions (3.3), lead to the following result: A non-trivial solution of (3.2) - (3.4)

is given implicitly by

$$
\begin{aligned}
& x = I(v;\ v_e,\ v_o) \\
(3.9) \qquad & u = c\left[\frac{v_e - v_o}{2}\right]^{-1/2}\left[(v-v_o)C(v_e,\ v_o) - (v_e-v_o)C(v,\ v_o)\right]^{1/2} ,
\end{aligned}
$$

provided there exists a $v_e > v_o$ such that

$$(3.10) \qquad a = I(v_e;\ v_e,\ v_o) \quad ,$$

and

$$(3.11) \qquad \frac{C(\xi,\ v_o)}{\xi - v_o} \leq \frac{C(v_e,\ v_o)}{v_e - v_o} \quad \text{for} \quad v_o \leq \xi \leq v_e \quad .$$

The constant solution, $u = 0$, $v = v_o$, is unique if there does not exist a number $v_e > v_o$ such that (3.10) and (3.11) are satisfied. If there exists only one such number, then there is only one non-trivial solution, and it is given by (3.9).

A sufficient condition for the uniqueness of a non-constant steady state is that $I(v;\ v,\ v_o)$ be an increasing function of v in the range $v > v_o$. For such cases condition (3.10) requires that

$$(3.12) \qquad a > \lim_{v_e \to v_o} I(v_e;\ v_e,\ v_o) \quad .$$

This limit is obtained by introducing

$$
\begin{aligned}
& \varepsilon = v_e - v_o \\
(3.13) \qquad & \xi = \varepsilon\eta + v_o \quad ,
\end{aligned}
$$

into (3.8) to obtain

$$I(v_e; v_e, v_o) = I(v_o + \varepsilon; v_o + \varepsilon, v_o)$$

$$(3.14) \qquad = \frac{\varepsilon}{\sqrt{2}} \int_0^1 \left[\eta C(v_o + \varepsilon, v_o) - C(v_o + \varepsilon\eta, v_o)\right]^{-1/2} d\eta .$$

A Taylor-series expansion gives

$$C(v_o + \varepsilon\eta, v_o) = \frac{\varepsilon^2\eta^2}{2} A(v_o) + \frac{\varepsilon^3\eta^3}{6} A'(v_o + \theta\varepsilon\eta) , \quad o \le \theta \le 1 ,$$

where we have used the definitions (3.6) and (3.7). Using this result in (3.14) and passing to the limit yields

$$\lim_{v_e \to v_o} I(v_e; v_e, v_o) = \frac{1}{\sqrt{A(v_o)}} \int_0^1 \frac{d\eta}{\sqrt{\eta(1-\eta)}}$$

$$= \pi/\sqrt{A(v_o)} \qquad .$$

Thus condition (3.12), which is necessary for the existence of a non-trivial steady state in the present case, becomes

$$(3.15) \qquad a > \pi/\sqrt{A(v_o)} \qquad .$$

In terms of the dimensional variables this condition is simply $k_{ex}(v_o) > o$. If $I(v; v, v_o)$ is a decreasing function of v for $v > v_o$, the above condition with the inequality reversed is necessary for uniqueness.

The condition (3.11) has a simple geometric interpretation. Consider the curve $y = C(\xi, v_o)$ for $\xi \geq v_o$. Then v_e must be a number $> v_o$ such that this curve lies below the line with slope $C(v_e, v_o)/(v_e - v_o)$, passing through the point $\xi = v_o$, $y = 0$. From formula (3.9) this slope can be shown

to have the interpretation

$$(3.16) \qquad \frac{C(v_e,\ v_o)}{v_e - v_o} = v''(o) \geq o \quad .$$

The non-negativeness results from the fact that $\frac{dy}{d\xi} = 0$ at $\xi = v_o$. Similarly we deduce from (3.11)

$$(3.17) \qquad \left.\frac{dy}{d\xi}\right|_{\xi = v_e} = B(v_e,\ v_o) \geq \frac{C(v_e,\ v_o)}{v_e - v_o} \quad .$$

The conditions (3.16) and (3.17) are helpful in attempting to verify (3.11) for a specific problem. The former may also be used as a convergence criterion in numerical work.

As an important illustration of the above results we consider the case $A(\xi) = 1 - \xi$. Then from definitions (3.6) and (3.7)

$$(3.18) \qquad \begin{aligned} B(v,\ v_o) &= \tfrac{1}{2}\,(v-v_o)(2-v_o-v) \\ C(v,\ v_o) &= \tfrac{1}{6}\,(v-v_o)^2(3-2v_o-v) \quad . \end{aligned}$$

Since, from (3.16) and (3.17), $B(v_e,\ v_o) \geq o$, and since for non-trivial steady states $v_e > v_o$, we may deduce from the first equation of (3.18)

$$(3.19) \qquad v_o < 1 \quad .$$

This is a necessary condition for the existence of a non-constant steady state. Then condition (3.11) is satisfied provided

$$(3.20) \qquad v_o < v_e \leq \frac{3-v_o}{2} \quad ,$$

which furnishes a bound on the steady-state exit-temperature. The above inequality is easily obtained by using (3.18) and (3.19) in (3.17). The integral in equation (3.10) becomes in the present case

$$(3.21) \qquad I(v_e;\ v_e,\ v_o) = \int_0^1 \left[\eta(1-\eta)(1-v_o - \tfrac{\varepsilon}{3}[1+\eta])\right]^{-1/2} d\eta ,$$

where $\varepsilon = v_e - v_o$. This is obviously an increasing function of ε and hence of v_e. Therefore we require from condition (3.15)

$$(3.22) \qquad a > \pi/\sqrt{1-v_o} \qquad .$$

From (3.21) we see that $I(v_e;\ v_e,\ v_o) \longrightarrow \infty$ as $v_e \longrightarrow \frac{3-v_o}{2}$ and hence a unique non-constant steady state exists for any $a > \pi/\sqrt{1-v_o}$ and $v_o < 1$. Using (3.18) in (3.9) this solution is obtained in terms of an elliptic function. For the case $v_o = 0$, the solution has been given by J. Fleck [1].

Section 4. Temperature Bounds*

Let u(t, x), v(t, x) be solutions of (2.10) satisfying the boundary conditions (2.7) and initial conditions (2.11-2.13). We first prove that $u(t, x) \geq 0$ which justifies (3.4) and is used later. The proof uses the following form of the weak maximum principle for parabolic equations: Let w(t, x) be a solution of the equation

$$(4.1) \qquad w_t = w_{xx} + \phi(t, x)w$$

* This section is an adaptation, in somewhat less rigorous form, of a forthcoming paper [3].

in the rectangle

(4.2) $\quad R_T\colon\ o \le x \le a \quad , \quad o \le t \le T \quad .$

If $\phi(t, x) \le o$ and $w(t, x) \ge o$ in R_T, then w attains its maximum on one of the boundary segments

(4.3) $\quad x = 0,\ t = 0,\ \text{or } x = a \quad .$

This principle has long been known in various forms; see for example M. Picone [ ].

In the rectangle R_T of (4.2) we define

$$w(t, x) = e^{-\lambda t}u(t, x)$$

where

$$\lambda \equiv \lambda(T) = \max A(v(t, x)), \text{ for } (t, x) \in R_T \quad .$$

Then w satisfies (4.1) with $\phi(t, x) = A(v) - \lambda \le o$ in R_T. From the above maximum principle we may conclude that w, and therefore u, assume negative values in R_T only if u assumes a negative minimum on one of the segments (4.3). But u, and therefore w, are $\ge o$ on (4.3) by the conditions (2.7a), (2.11a) and (2.12). Therefore $u \ge o$ in R_T and since T is arbitrary $u(t, x) \ge o$ for all $t \ge o$.

To obtain bounds for $v(t, x)$ we consider the rectangle R_T as the sum of four boundaries and the interior as follows:

$$\begin{array}{lllll}
 & N\colon & o < x < a & , & t = T \\
 & E\colon & x = a & , & o < t \le T \\
(4.4) & S\colon & o \le x \le a & , & t = 0 \\
 & W\colon & x = 0 & , & o < t < T \\
 & I\colon & o < x < a & , & o < t < T \quad .
\end{array}$$

We also define sets R_T^- and R_T^+ as the intersections of R_T with the half planes $ct - x \leq o$ and $ct - x > o$ respectively.

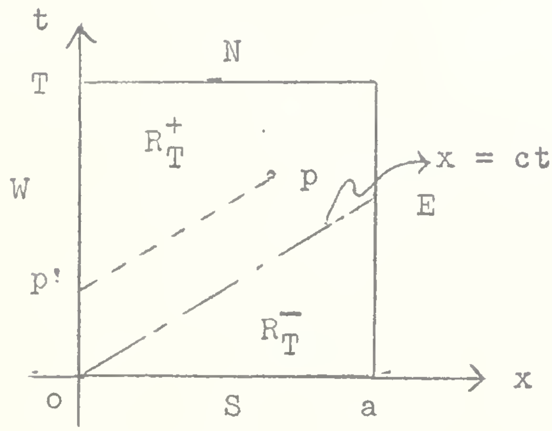

Figure 1.

A lower bound is found immediately by considering the segments of slope $^1/c$ from each point p of R_T to a corresponding point p' on W or S. Since $u(t, x) \geq o$ it follows by integration of (2.10b) along these segments that $v(p) \geq v(p')$. However, from (2.7b) and (2.11b) we have $v(p') = v_o$ on W and $v(p') \geq \alpha \equiv \min g(x)$ on S. Thus,

$$
(4.5) \qquad \begin{aligned} v(p) &\geq v_o \quad \text{for } p \varepsilon R_T^+ \\ v(p) &\geq \alpha \quad \text{for } p \varepsilon R_T^- \end{aligned} \quad ,
$$

or since $g(o) = v_o$ we have

$$
(4.6) \qquad v(p) \geq \alpha \text{ for } p \varepsilon R_T
$$

To obtain an upper bound on v we eliminate u from (2.10) and get

$$
(4.7) \quad \left\{ \frac{\partial}{\partial t} + c \frac{\partial}{\partial x} \right\} \left[-v_t + v_{xx} + B(v, v_o) \right] = 0 \quad ,
$$

where $B(v, v_o)$ is defined by (3.6). This equation implies that

$$(4.8) \qquad v_t = v_{xx} + B(v, v_o) + F(ct-x)$$

for some continuous function F. To obtain an upper bound on v we require an upper bound on F. Thus setting t = 0 in (4.8) we get on S

$$(4.9) \qquad \begin{aligned} F(-x) &= v_t(o, x) - v_{xx}(o, x) - B(v(o, x), v_o) \\ &= f(x) - cg'(x) - g''(x) - B(g(x), v_o) \quad , \end{aligned}$$

where we have used (2.10b) and the initial conditions (2.11). If we define γ by

$$(4.10) \qquad \gamma = \min_{o \le x \le a} [-f(x) + cg'(x) + g''(x) + B(g(x), v_o)] \quad ,$$

then (4.9) yields

$$(4.11) \qquad F(ct-x) \le - \gamma \text{ for } (t, x) \varepsilon R_T^- \quad .$$

For positive arguments we set x = 0 in (4.8) and obtain on W

$$(4.12) \qquad \begin{aligned} F(ct) &= v_t(t, o) - v_{xx}(t, o) - B(v(t, o), v_o) \\ &= - v_{xx}(t, o) \quad . \end{aligned}$$

Here we have used (2.7b) to get $v_t(t, o) = 0$ and, with the definition (3.6), $B(v_o, v_o) = 0$. Since, from (2.7a), $u(t, o) = 0$ and as above $v_t(t, o) = 0$ we get $v_x(t, o) = 0$ from (2.10b). However, (4.5) requires that $v \ge v_o$ in a neighborhood of each point of W, and thus

$$v_{xx}(t, o) \ge o \quad .$$

This result and (4.12) require

$$(4.13) \qquad F(ct-x) \le o \text{ for } (t, x) \varepsilon R_T^+ \quad ,$$

which together with (4.11) furnish the required bounds on F in R_T.

Let P be a point of R_T at which v attains its maximum value. Then P lies in one of the continua E, S, W, or $N + I$. If $P \epsilon W$, then $v(P) = v_o$ by the boundary condition (2.7b). This is, in a sense, a trivial case as then $v(t, x) = v_o$ for $(t, x) \epsilon R_T^+$, by (4.5). If $P \epsilon S$, then by the initial condition (2.11b)

$$v(P) = \beta \equiv \max_{o \leq x \leq a} g(x) \quad . \tag{4.14}$$

Suppose $P \epsilon N + I$; then since $v(P)$ is a maximum and the set $N + I$ is open with respect to x and open from below with respect to t, we must have

$$v_x(P) = 0, \ v_{xx}(P) \leq o, \ v_t(P) \geq o \ . \tag{4.15}$$

Taking (4.8) at this point P yields

$$B(v(P), v_o) + F(P) \geq o \quad ,$$

or from the bounds (4.11) and (4.13) on F

$$\begin{aligned} B(v(P), v_o) &\geq \begin{cases} \gamma \text{ for } P \epsilon R_T^- \\ o \text{ for } P \epsilon R_T^+ \end{cases} \quad , \text{ or in general} \\ &\geq \min(\gamma, o) \text{ for } P \epsilon N + I \ . \end{aligned} \tag{4.16}$$

If there exists an $M \geq v_o$ such that

$$\begin{aligned} &B(M, v_o) = \min(\gamma, o) \\ &B(v, v_o) < \min(\gamma, o) \text{ for } v > M \end{aligned} \tag{4.17}$$

we could conclude from (4.16) that

(4.18) $\quad v(P) \leq M$.

Since $B(v_o, v_o) = 0$, and $B(v, v_o)$ is a continuous function of v, (4.17) is implied by the condition

(4.19) $\quad \limsup_{v \to \infty} B(v, v_o) < \min(\gamma, o)$.

We assume this condition to hold, which is a restriction on the given function A(v), and hence (4.18) follows.

Finally, suppose $P \epsilon E$. Since v(P) is the maximum value of v, the definition (4.4) of E leads to the inequalities

$$v_x(P) \geq o, \; v_t(P) \geq o \; .$$

But $v_t + cv_x = u = 0$ on E, and c is > o . Therefore the above inequalities yield

(4.20) $\quad v_x(P) = 0, \; v_t(P) = 0$.

From the maximum property of v(P) we may now conclude

(4.21) $\quad v_{xx}(P) \leq o$.

From (4.20) and (4.21) follow (4.15) and, hence, the inequality $v(P) \leq M$. Summarizing the results for all four sets E, S, W, and N + I we find $v(P) \leq \max(\beta, M)$ regardless of where the maximum value v(P) is attained in R_T. However, since T is arbitrary we have obtained a bound for all $t \geq o$. Thus we have proven the following:

Theorem. Let u(t, x), v(t, x) be a solution of (2.10) satisfying the boundary conditions (2.7) and initial conditions

(2.11 - 2.13). Let $B(v, v_o)$ satisfy condition (4.19). Then $u(t, x) \geq o$ and $v(t, x)$ is bounded for all $t \geq o$ and $o \leq x \leq a$; v satisfies the inequality

$$(4.22) \qquad \alpha \leq v(t, x) \leq \max(\beta, M) \quad ,$$

where $\alpha = \min g(x)$, $\beta = \max g(x)$, and M is defined by (4.17).

As an explicit application of the above theorem we consider the case $A(v) = 1 - v$. The corresponding $B(v, v_o)$ is given in (3.18). We see that $\lim_{v \to \infty} B(v, v_o) = -\infty$ so that (4.19) is satisfied for all γ and v_o. The number M of condition (4.17) is easily found to be

$$(4.23) \qquad M = \begin{cases} v_o & \text{for } \gamma \geq o,\ v_o \geq 1 \\ 2-v_o & \text{for } \gamma \geq o,\ v_o \leq 1 \\ 1 + [(1-v_o)^2-2\gamma]^{1/2} & \text{for } \gamma < o \quad . \end{cases}$$

Section 5. Numerical Solution

We consider the equations

$$(5.1) \qquad \begin{aligned} &a) \quad R[u, v] \equiv v_t + cv_x - u = 0 \\ &b) \quad S[u, v] \equiv u_t - u_{xx} - \phi(u, v) = 0 \end{aligned}$$

subject to the boundary and initial conditions

$$(5.2) \qquad \left.\begin{aligned} u(o, t) = u(a, t) = 0 \\ v(o, t) = v_o \end{aligned}\right\} t > o \ ; \quad \left.\begin{aligned} u(x, o) = f(x) \\ v(x, o) = g(x) \end{aligned}\right\} o \leq x \leq a \ .$$

Equations (5.1) are more general than those of (2.10), and the restrictions (2.12) and (2.13) on the initial data have been dropped. We assume the existence of a unique solution to the above problem. In the present section we associate a system of finite-difference equations with (5.1) and show that they

have a unique solution.

On the rectangle R_T of (4.2) we introduce the mesh

$$(5.3)\qquad \begin{cases} x_i = ih \\ t_j = jk \end{cases}, \quad \text{where} \quad \begin{cases} h = {}^a/_N \\ k = {}^T/_J \end{cases},$$

and N and J are fixed positive integers. Let U_i^j, V_i^j be defined on the mesh as solutions of the difference equations

(5.4)

a)

$$\left.\begin{aligned} &kR_h[U_i^j, V_i^j] \equiv (V_i^j - V_i^{j-1}) + \mu(V_i^{j-1} - V_{i-1}^{j-1}) - kU_i^{j-1} = 0 \qquad , 1 \le i \le N \\ &\text{b)} \\ &kS_h[U_i^j, V_i^j] \equiv (U_i^j - U_i^{j-1}) - \lambda(U_{i+1}^j - 2U_i^j + U_{i-1}^j) - \emptyset(U_i^{j-1}, V_i^{j-1}) = 0, 1 \le i \le N-1 \end{aligned}\right\} 1 \le j \le J$$

where

$$(5.5)\qquad \left.\begin{aligned} U_o^j &= U_N^j = 0 \\ V_o^j &= v_o \end{aligned}\right\} j \ge 1 \quad ; \qquad \left.\begin{aligned} U_i^o &= f(x_i) \\ V_i^o &= g(x_i) \end{aligned}\right\} o \le i \le N .$$

In (5.4) we have introduced

$$(5.6)\qquad \mu \equiv c\,{}^k/_h \quad , \quad \lambda \equiv {}^k/_{h^2} \quad .$$

The solution of these equations is easily obtained by induction. Thus we assume $U_i^{j'}$, $V_i^{j'}$ known for all $j' \le j - 1$. From (5.4) a) we have

$$V_i^j = (1-\mu)V_i^{j-1} + \mu V_{i-1}^{j-1} + kU_i^{j-1} \qquad , \quad 1 \le i \le N$$

which uniquely determines the V_i^j . We write (5.4) b) as

$$\lambda U_{i+1}^j - (1+2\lambda)U_i^j + \lambda U_{i-1}^j = - U_i^{j-1} - \emptyset(U_i^{j-1}, V_i^{j-1}), \; 1 \le i \le N - 1 .$$

This is a system of N - 1 equations for as many unknowns, since

$U_o^j = U_N^j = 0$ by (5.5). The coefficient matrix is non-singular, which insures a unique solution of this system of equations. For computational purposes this matrix may be factored into a product of a lower - by an upper - triangular matrix. The solution is then obtained by evaluating a pair of two-term recursions.

If the last term in (5.4) b) is taken at j, rather than j - 1, the resulting implicit equations would, in general, not be linear. However, they could be solved by an iteration scheme the convergence of which has been examined by M.E.Rose[4].

Section 6. Convergence and Error Estimate

Let $u(x, t)$, $v(x, t)$ be the unique solution of (5.1) and (5.2) in R_T and U_i^j, V_i^j be the solution of (5.4) and (5.5) on the mesh (5.3). We define the error of the numerical solution as

$$E_i^j = U_i^j - u(x_i, t_j)$$
(6.1)
$$F_i^j = V_i^j - v(x_i, t_j)$$

In the present section we shall prove that the condition

(6.2) $\quad \mu \equiv c^k/h < 1$

is sufficient to insure the uniform boundedness of $|E_i^j|$ and $|F_i^j|$. The bounds are such that if $h \longrightarrow o$ and $k \longrightarrow o$ while maintaining condition (6.2), then the error uniformly approaches zero.

The above results will follow from the boundedness of the solution, X_i^j, Y_i^j of the following set of linear differ-

ence equations on the mesh (5.3):

(6.3)

a)

$$R_h[X_i^j, Y_i^j] = r_i^j \quad , \quad 1 \le i \le N$$

b) $\qquad 1 \le j \le J$

$$L_h[X_i^j, Y_i^j] = \ell_i^j \quad , \quad 1 \le i \le N-1$$

c)

$(X_o^j, Y_o^j, X_N^j, X_i^o, Y_i^o)$ = given, for $1 \le j \le J$ and $o \le i \le N$.

Here R_h is defined as in (5.4) a) and

(6.4)

$$kL_h[X_i^j, Y_i^j] \equiv (X_i^j - X_i^{j-1}) - \lambda(X_{i+1}^j - 2X_i^j + X_{i-1}^j) - a_i^{j-1}X_i^{j-1} - b_i^{j-1}Y_i^{j-1} \quad .$$

The condition (6.2) is assumed to hold for the mesh (5.3).

To prove the boundedness of the X_i^j and Y_i^j we introduce:

(6.5)

a)

$$A \equiv \max_{ij}|a_i^j|, \; B \equiv \max_{ij}|b_i^j| \quad ;$$

b)

$$\xi \equiv \max_{ij}(|r_i^j|, |\ell_i^j|, |X_i^o|, |Y_i^o|, |X_o^j|, |Y_o^j|, |X_N^j|) \quad ;$$

c)

$$X_j \equiv \max_i(|X_i^j|, \xi) \quad , \quad Y_j \equiv \max_i(|Y_i^j|, \xi) \quad ;$$

d)

$$\overline{X}_j \equiv \max_{j' \le j} X_{j'} \quad , \quad \overline{Y}_j \equiv \max_{j' \le j} Y_{j'} \quad ,$$

Then solving (6.3) a) for Y_i^j, taking absolute values, and using (6.5) b) and c) we obtain, since $\mu < 1$,

$$|Y_i^j| \le Y_{j-1} + kX_{j-1} + k\xi \quad , \quad 1 \le i \le N \quad ,$$

By definition we have $Y_{j-1} \geq \xi$ and thus

$$Y_j \leq Y_{j-1} + kX_{j-1} + k\xi \quad .$$

Applying this inequality recursively yields, with the aid of (6.5) b) and d)

$$(6.6) \qquad Y_j \leq jk\bar{X}_{j-1} + (1+jk)\xi \quad .$$

This furnishes a bound on the Y_i^j in terms of a bound on the $X_i^{j'}$ for $j' < j$. To obtain the latter bound we write (6.3) b) as

(6.7)

$$(X_i^j - X_i^{j-1}) - \lambda(X_{i+1}^j - 2X_i^j + X_{i-1}^j) = k(a_i^{j-1}X_i^{j-1} + b_i^{j-1}Y_i^{j-1} + \ell_i^j), \quad 1 \leq i \leq N-1.$$

From (6.5) b) and c) either

$$(6.8) \qquad X_j = \xi \quad \text{or} \quad X_j = \max_{1 \leq i \leq N-1} |X_i^j| > \xi$$

Assume the latter case to hold and let i, $1 \leq i \leq N-1$, be a subscript for which $X_j = |X_i^j|$. If $X_i^j > 0$ we have from (6.7)

$$(X_i^j - X_i^{j-1}) \leq k(a_i^{j-1}X_i^{j-1} + b_i^{j-1}Y_i^{j-1} + \ell_i^j) \quad ,$$

or using (6.5) a)-c),

$$(X_i^j| \leq |X_i^{j-1}| + k(A|X_i^{j-1}| + B|Y_i^{j-1}| + \xi)$$

(6.9)

$$\leq (1+kA)X_{j-1} + kBY_{j-1} + k\xi \quad .$$

If $X_i^j < 0$, (6.7) yields

$$(X_i^j - X_i^{j-1}) \geq k(a_i^{j-1}X_i^{j-1} + b_i^{j-1}Y_i^{j-1} + \ell_i^j) \quad ,$$

or on multiplication by -1,

$$-X_i^j \leq -X_i^{j-1} - k(a_i^{j-1}X_i^{j-1} + b_i^{j-1}Y_i^{j-1} + \ell_i^j) \quad .$$

Since, in this case, $-X_i^j > o$, we may take absolute values in the above inequality and obtain again (6.9). By definition $X_{j-1} \geq \xi$, and thus (6.9) yields in either of the cases (6.8)

$$X_j \leq (1+kA)X_{j-1} + kBY_{j-1} + k\xi \; .$$

From (6.6) in the above inequality and since $\overline{X}_{j-1} \geq \overline{X}_{j-2}$ we obtain

$$(6.10) \qquad X_j \leq (1+kA)X_{j-1} + kB(j-1)k\overline{X}_{j-1} + [1+B+B(j-1)k]k\xi$$

Since (6.10) holds for each j in $1 \leq j \leq J$ we have, using (6.5) d)

$$\overline{X}_j \leq (1+kA+kBt_j)\overline{X}_{j-1} + (1+B+Bt_j)k\xi \; , \; t_j = jk \quad .$$

Applying this inequality recursively and taking $j = J$ we obtain

$$(6.11) \qquad \overline{X}_J \leq \left\{ [1+k(A+BT)]^J + \frac{[1+k(A+BT)]^J-1}{(A+BT)}[1+B+BT] \right\} \xi \quad .$$

From (6.5) d) and the above result, (6.6) implies

$$(6.12) \qquad \overline{Y}_J \leq T\overline{X}_{J-1} + (1+T)\xi \quad .$$

These are the required uniform bounds for X_i^j and Y_i^j on the mesh (5.3). A useful form of (6.11) is obtained by setting $k = {}^T/J$ and using

$$(1+ {}^{\alpha}/n)^n < e^{\alpha} \text{ for } n, \alpha > o \quad ;$$

thus

$$(6.13) \qquad \overline{X}_J \leq \left\{ e^{(A+BT)T} + \frac{e^{(A+BT)T}-1}{(A+BT)} (1+B+BT) \right\} \xi$$

From the definition (6.1) of the error and (5.1) a), (5.4) a) we have

$$R_h(E_i^j,\ F_i^j) = R_h(U_i^j,\ V_i^j) - R_h(u(x_i,\ t_j),\ v(x_i,\ t_j))$$

$$= R(u(x_i,\ t_j), v(x_i,\ t_j)) - R_h(u(x_i,\ t_j), v(x_i, t_j)).$$

From the usual Taylor expansions this becomes

(6.14)

$$R_h(E_i^j, F_i^j) = r_{ij} = \frac{k}{2} v_{tt}(x_i, t_j - \theta_1 k) + \frac{h}{2} v_{xx}(x_i - \theta_2 h, t_j) \ ; \ 0 \le \theta_1, \theta_2 \le 1$$

Similarly we obtain from (5.1) b), (5.4) b) and (6.1)

(6.15)

$$L_h(E_i^j, F_i^j) = \ell_{ij} = -\frac{k}{2} U_{tt}(x_i, t_j - \theta_1 k) - \frac{h^2}{12} u_{xxxx}(x_i + \theta_2 h, t_j), 0 \le \theta_1, \theta_2 \le 1;$$

where

(6.16)

$$\left.\begin{aligned} a_{ij} &= \frac{\partial \phi}{\partial u}(\bar{u}_i^j,\ \bar{v}_i^j) \\ b_{ij} &= \frac{\partial \phi}{\partial v}(\bar{u}_i^j,\ \bar{v}_i^j) \end{aligned}\right\{ \begin{aligned} \bar{u}_i^j &= \theta_i^j U_i^j + (1-\theta_i^j) u(x_i,\ t_j) \\ \bar{v}_i^j &= \phi_i^j V_i^j + (1-\phi_i^j) v(x_i,\ t_j) \end{aligned} \quad , \ 0 \le \theta_i^j, \phi_i^j \le 1$$

On the boundary of the mesh (5.3) we have

$$(6.17) \left\{ \begin{aligned} &E_i^0 = F_i^0 = 0 \ , \quad 0 \le i \le N \\ &E_0^j = F_0^j = E_N^j = 0 \ , \quad 0 \le j \le J \ . \end{aligned} \right.$$

Thus the error satisfies a system of equations formally identical to (6.3). If condition (6.2) is satisfied then the bounds (6.12) and (6.13) apply to $|F_i^j|$ and $|E_i^j|$ respectively, where now

(6.18)

$$A = \max_{ij}\left|\frac{\partial \phi(\bar{u}_i^j, \bar{v}_i^j)}{\partial u}\right| \quad , \quad B = \max_{ij}\left|\frac{\partial \phi(\bar{u}_i^j, \bar{v}_i^j)}{\partial v}\right|$$

$$\xi = k/2 \max_{ij}\left(\left|v_{tt}(x_i, \bar{t}_j) + \frac{c}{\mu} v_{xx}(\bar{x}_i, t_j)\right|, \left|u_{tt}(x_i, \bar{t}_j) + k\frac{c^2}{\mu^2} u_{xxxx}(\bar{x}_i, t_j)\right|\right)$$

Here the arguments are understood to be those of (6.14), (6.15) and (6.16). For any value of t, say t = T, we may consider a sequence of meshes (5.3) such that $k \longrightarrow o$, while Jk = T and $\mu < 1$ in each mesh. Then the bounds (6.12) and (6.13) hold in each mesh but, from (6.18), $\xi \longrightarrow o$. Thus the error approaches zero and hence the numerical solution uniformly converges to the solution of the partial differential equations (5.1) in R_T .

For the difference scheme mentioned at the end of Section 5 we must add to (6.2) the condition

(6.19) $$kA < 1 \quad .$$

Then by the above arguments it can be shown that the identical bounds (6.12) and (6.13) hold for the error, and hence the uniform convergence of this scheme is also established.

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